Hydrogen atom injection into carbon surfaces by comparison between Monte-Carlo, molecular dynamics and ab-initio calculations

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To understand the plasma-wall interaction on divertor plates, we investigate the interaction of hydrogen atoms and carbon materials used in the high heat flux components by the use of the following simulations. Monte-Carlo (MC) method based on binary collision approximation can calculate the sputtering process of hydrogen atoms on the carbon material quickly. Classical molecular dynamics (MD) method employs multi-body potential models and can treat realistic structures of crystal and molecule. The *ab-initio* method can calculate electron energy in quantum mechanics, which is regarded as realistic potential for atoms.

In the present paper, the interaction of the hydrogen and the carbon material is investigated using the multi-scale (MC, MD and *ab-initio*) methods. The bombardment of hydrogen atoms onto the carbon material is simulated by the ACAT-code of the MC method, which cannot represent the structure of crystal, and the MD method using modified reactive empirical bond order (REBO) potential, which treats single crystal graphite and amorphous carbon. Consequently, we clarify that the sputtering yield and the reflection rate calculated by the ACAT-code agree with those on the amorphous carbon calculated by the MD. Moreover, there are many kinds of REBO potential for the MD. Adsorption, reflection and penetration rates between a hydrogen atom and a graphene surface are calculated by the MD simulations using the two kinds of potential model. For the incident energy of less than 1 eV, the MD simulation using the modified REBO potential, which is based on Brenner's REBO potential in 2002, shows that reflection is dominant, while the most popular Brenner's REBO potential in 1990 shows that adsorption is dominant. This reflection of the low energy injection is caused by a small potential barrier for the hydrogen atom in the modified REBO potential. The small potential barrier is confirmed by the *ab-initio* calculations, which are hybrid DFT (B3LYP/cc-pVDZ), *ab-initio* (RCCSD(T)/cc-pVDZ), and G2MS levels of theory.